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Special States in the Spin–Boson Model

L. S. Schulman[1]

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For the spin–boson model we numerically exhibit special microscopic initial states that evolve, under pure quantum dynamics, from one macroscopically well-defined state to another. This is unusual in that typical states of the model evolve to superpositions of macroscopically different states. Although the mathematical rationale for the existence of the special states is not clear, that existence reflects favorably on a proposed theory of quantum measurement.

KEY WORDS: Spin–boson model; quantum measurement theory; quantum decay.

1. INTRODUCTION

Several interrelated issues are addressed here. At the mathematical level we report the existence of special microscopic states of a "large" system having the property that their dynamical evolution leads to outcomes different from those of typical microscopic states. Physically, the existence of these "special" states reflects favorably on a proposed statistical mechanics-based resolution of the problems of quantum measurement theory.[1] That resolution is based on microscopic states of a system (including apparatus and environment) which under exact microscopic time evolution lead to microscopic states that correspond to a *single* macroscopic state, rather than (as in "cat" experiments) to superpositions of macroscopically different states. With such "special" states as initial conditions there is no longer the problem of eliminating or explaining away the multiplicity of macroscopically possible outcomes, but there are other questions, particularly regarding why nature should select rare initial conditions. For those questions and for their relation to the foundations of statistical

[1] Physics Department, Clarkson University, Potsdam, New York 13699-5820.

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mechanics see ref. 1. This article is concerned with the technical issue of the existence of "special" states.

That issue is not trivial, even beyond the occasional difficulty of identifying degrees of freedom for the "specializing." The states may also be required to *dis*entangle. Only recently—via EPR-type experiments—has the profound effect of wave function entanglement begun to be explored, although Schrödinger long ago described entanglement as *the* essential feature of quantum mechanics.[2] In the von Neumann formulation, pure quantum evolution [i.e., $\psi \rightarrow \exp(-iHt)\psi$] only seems to entangle more and more, with disentanglement occurring by collapse (or whatever). In the theory of ref. 1, which allows only pure quantum evolution, there must be *dis*entanglement as well as entanglement.

In this article we study the spin–boson model. It is not the full Hamiltonian of some large apparatus, but it has been extensively used for the realistic description of practical, physical systems. It has played a prominent role in the study of Josephson junctions, including situations where quantum measurement-related issues arise. But it has also been applied to other systems, and serves at the intersection of classical mechanics (as a model of dissipation), quantum mechanics, and statistical mechanics.[3–5]

2. THE SPIN–BOSON MODEL

The Hamiltonian is

$$H = \varepsilon\left(\frac{1+\sigma_z}{2}\right) + \Delta\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \sigma_z \sum_k \beta_k (a_k^\dagger + a_k) + \sum_k \frac{\beta_k^2}{\omega_k} \tag{2.1}$$

where the two-level "spin" operators are the matrices σ_z and σ_x, the bosons have frequencies ω_k, the spin–boson coupling is proportional to β_k, the up–down coupling is given by Δ, and the unperturbed level energy difference is ε.

A "special" state is manifested in this context in the following way. The observed variable is the spin state, up or down. The microscopic variables are the bosons. Fix a time T during which the system is supposed to evolve under the Hamiltonian (2.1) only, and subsequent to which it is coupled to a larger environment. In this article we assume that it is the larger environment that fixes the spin–boson oscillations irreversibly. Using thermal averaging or other bland initial conditions, the system would go from an initial up state to a superposition of up and down states at that later time T. This would be a "grotesque" state whose potential existence is at the heart of the quantum measurement problem. The claim of ref. 1 is that there are particular—not "bland," but "special"—initial boson states such that the state at time T is entirely spin-up, and other "special" states such that it is entirely down.

Information about such states can be extracted as follows: The initial state $|\phi_0\rangle$ is of the form

$$|\phi_0\rangle = |+\rangle \otimes \sum A_{\{n_k\}} \, |n_{k_1}, n_{k_2}, \ldots\rangle$$

Under the full Hamiltonian it evolves to $|\phi_T\rangle = \exp(-iHT)\,|\phi_0\rangle$. The physically important quantity is the norm (squared) of the portion of the vector that remains "up." In ordinary parlance this is the probability of nondecay. The Hilbert space consists of tensor products of boson states and up and down spin states. Let P be the projection on the subspace with spin up. We define $p_T \equiv \|P\,|\phi_T\rangle\|^2$.

The existence of a "special" state corresponds to states $|\phi_0\rangle$ for which p_T is either zero or one. As discussed in ref. 1, we seek states for which that quantity can be made close to those ideals. We rewrite p_T,

$$\begin{aligned} p_T &\equiv \langle (P\phi_T) \,|\, P\phi_T\rangle = \langle \phi_0|\, \exp(iHT)\, PP \exp(-iHT)\, |\phi_0\rangle \\ &= \langle \phi_0|\, A_T^\dagger A_T \,|\phi_0\rangle = \langle \phi_0|\, B_T \,|\phi_0\rangle \end{aligned}$$

where we have used $|\phi_0\rangle = P\,|\phi_0\rangle$, and have defined

$$A_T \equiv P\exp(-iHT)P, \qquad B_T \equiv A_T^\dagger A_T$$

It follows that the existence of "special" states is equivalent to the existence of spin-up eigenvectors with eigenvalues zero or one of the operator B_T. It is easy to see that the eigenvalues of B_T lie in the interval $[0, 1]$.

3. ANALYTIC METHODS

A "special" state solves a two-time boundary value problem in quantum mechanics.[6] Although remarks of Eddington on the interpretation of quantum mechanics led Schrödinger to consider two-time boundary value problems as early as 1932,[7] in fact what he looked at was the diffusion equation, not the *quantum* two-time boundary value problem. To formulate such a boundary value problem one may specify an initial state in a subspace $\mathscr{H}_1$ of Hilbert space and a final state in a subspace $\mathscr{H}_2$. If $n \equiv \dim(\mathscr{H}_1) + \dim(\mathscr{H}_2) - \dim(\mathscr{H}) > 0$, then there will be at least an n-dimensional family of solutions[2] (by parameter counting). However, the

[2] For given H and T, a "solution" is $\psi \in \mathscr{H}_1$ such that $\exp(-iHT)\psi \in \mathscr{H}_2$.

interesting case is where n is zero or negative and one manages a solution or near solution anyway. (Other two-time quantum boundary problems are given in refs. 8–10.)

The time dependence of the spin–boson model has been intensively studied.[3,5] The "blip" description is based on the same mathematical principle as Feynman's checkerboard path integral or Kac's treatment of the telegrapher equation.[11,12] Unfortunately, even with so much control I have not found a way to address the question of "special" states. Differential equation techniques can be useful,[13] but they have not been extended to this problem.

4. NUMERICAL RESULTS ON "SPECIAL" STATES

We study the eigenvalues of B_T numerically by truncating the Hilbert space. First we only consider a few bosons, and second they are given a cutoff by setting a maximum boson number N_{cutoff} (which may vary with ω). In general, reducing degrees of freedom makes the finding of "special" states *more* difficult.

In Fig. 1 we show the eigenvalues of B_T for various T for a Hamiltonian involving only a single boson. For Fig. 1 the Hamiltonian has

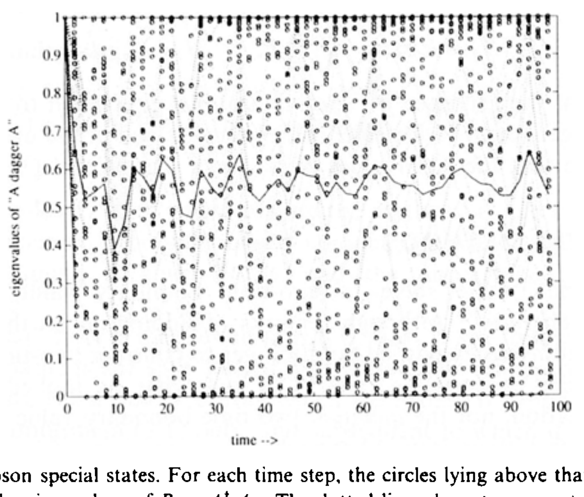


Fig. 1. One-boson special states. For each time step, the circles lying above that value of the time represent the eigenvalues of $B_T \equiv A_T^\dagger A_T$. The dotted lines do not represent the evolution of any particular individual state (a different set of eigenvectors occurs for each time step). The solid line is the average of the eigenvalues of B_T. States whose circles lie near the top of the graph represent special states for nondecay, and those near the bottom are special states for decay.

parameter values $\omega = 0.9$, $\varepsilon = 1$, $\Delta = 0.6$, and $\beta = 0.2$. The boson cutoff is $N \leqslant 31$.

The graph provides the following information: Note that at most times, for example, $T = 41$, there are points near 0 and near 1. As indicated, the time evolution is under a Hamiltonian with mode truncation, but which, for the remaining modes, contains the spin-up–spin-down couplings of Eq. (2.1). The points near 0 and 1 on the graph therefore mean that there are initial boson states such that, starting from spin up, they evolve to states that are almost entirely spin up at time 41 (this would correspond to a point near one, i.e., B_T has an eigenvalue near one). In addition, there are other time-zero boson states that leave the initial subspace almost entirely and decay to the spin-down state. These are the eigenfunctions of B_T with near-zero eigenvalues. ("Near" in Fig. 1 means a separation well below 10^{-3}.) The plotting of the spectrum of B_T for many values of T on the same graph—and the dotted line connecting eigenvalues at successive times—does not reflect the time dependence of any particular state. It is just that it is computationally convenient to generate many such spectra. Each T value plotted represents a different possible experiment. The remarkable feature shown is that there are *usually* such states. It is *not* exceptional to find "special" states.

Figure 2 shows the case of three-boson modes. Because the dimension increases rapidly in the tensor product, we take boson number cutoffs to be only 4, 3, and 3. The frequencies ω are respectively 0.1, 0.9, and 1.1, while $\beta = 0.2$ in all cases. The other parameters take the values $\varepsilon = 1$ and $\Delta = 0.5$. All points shown correspond to eigenvalues of B_T. Eigenvalues are now

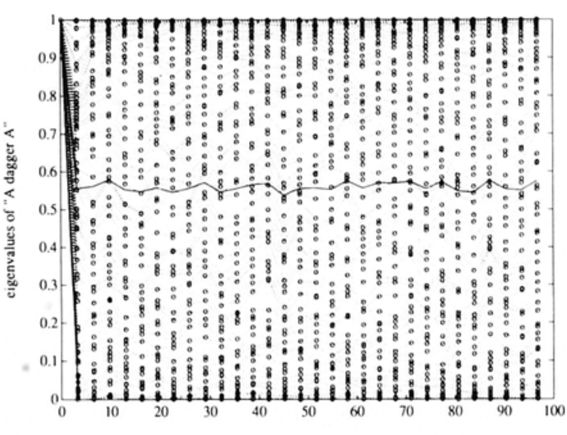


Fig. 2. Three-boson special states. The circles have the same interpretation as in Fig. 1.

even closer to 0 and 1 than for the one-boson case and in fact the density of eigenvalues near the extremes (0 and 1) appears to be greater than at the intermediate values.

For many, but not all, parameter values "special" states could be found. Exceptions can be generated, for example, by taking a single mode with $\omega = 2$; decay is substantially suppressed and "special" states for decay are not available. From the graph it can also be seen that "special" states are absent at very short times. This is a phenomenon related to dominated time evolution. We do not consider either absence to be a difficulty for the theory of ref. 1 and will explain below.

Remark. Some "special" states for nondecay are artifacts of the truncation, which in practice is an elimination of the coupling between N-boson states and $(N+1)$-boson states in the Hamiltonian. This can be seen by examining the actual "special" states and noting that in some cases they have large components near the cutoff. However, "special" nondecay states without this defect (as in the example given below) are also plentiful.

5. RATIONALE FOR THE "SPECIAL" STATES IN THE SPIN–BOSON MODEL

Although we are pleased to find this abundance of "special" states, the absence of an analytical demonstration is a drawback. For this reason we report further numerical investigation.

An instructive exercise is to look at the actual "special" states, the eigenvectors of B_T having near-zero and near-one eigenvalues. These are time-0 boson states having the property that at time T the spin state is all up or all down. In Fig. 3, we show two of the "special" states, the upper a "special" state for decay, with eigenvalue B_T near zero, and the lower a "special" state for nondecay, with the eigenvalue near 1. The abscissa is vector label, the first (left) half being $|+\rangle \otimes |k\rangle$, $k = 1,\ldots, N_{\text{cutoff}}$, and the second half being $|-\rangle \otimes |k\rangle$, with k in the same range. The ordinate is the absolute value of the amplitude for the state along the particular Hilbert space direction. Note that neither "special" state is large near the cutoff.

By applying $\exp(-iHt)$ to the initial state, one can watch it evolve, and in Figs. 4a and 4b we show the time development of the "special" state for decay. As a function of time, amplitude sloshes back and forth between the boson modes of the spin-up Hilbert subspace and those of the spin-down subspace. Representative times are shown. Notice that many boson modes simply do not participate. The "sloshing" involves a limited part of the Hilbert space. This is true for both the "special" state for decay (eigenvalue zero) and for nondecay. Except for the particular time of

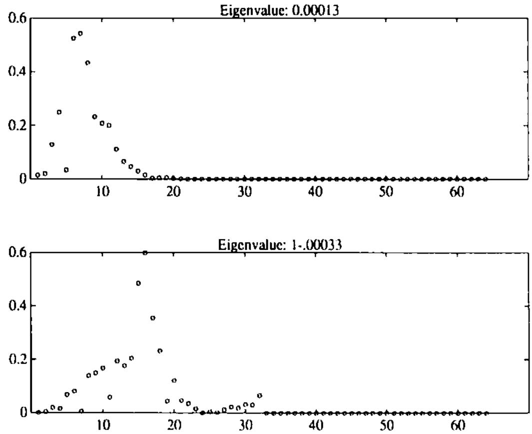


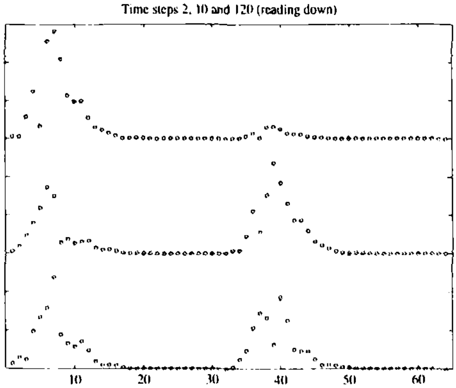
Fig. 3. "Special" states for decay (upper figure) and nondecay. These are eigenstates of B_T for $T \approx 33$. The 64×64 Hamiltonian (and thus the cutoff) is the same as that for Fig. 1 and its parameter values are given in the text. The initial state is entirely spin-up and therefore confined to the left entries in the figure (whose abscissa is vector label, as described in the text). Only the absolute value (*N.B.*: not its square) of the vector is shown.

"specializing," there is generally amplitude on both sides. Although space considerations prevent display of the time development of the nondecay "special" state, I can report that throughout its evolution it does not grow large near the cutoff.

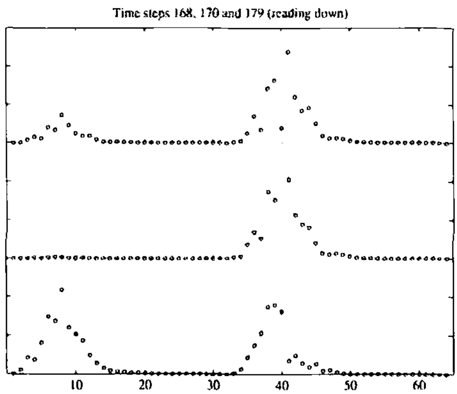
I believe that the limited use of directions in the Hilbert space plays a role in the successful search for "special" states in this model. The Hilbert subspaces associated with the initial and final states are each half the total Hilbert space dimension. Therefore with respect to parameter counting this is a borderline case. It seems though that by virtue of the particular dynamics there is less than the maximum spreading in Hilbert space. The initial vector remains in a small subspace[3] and the specification of the final space has a particular relation to that subspace, allowing exceptional or nongeneric "special" states to exist. This good fortune arises because both for the dynamics as well as for the characterization of the special states the same operator is involved, namely σ_z or, equivalently, the projection, P.

This is a kind of quantum localization. The relation of quantum localization to two-time boundary conditions was discussed in ref. 6 (see

[3] Strictly speaking, dynamical evolution under a unitary $\exp(-iHt)$ always leaves the dimension of the image unchanged. It is only when the overlap with less particularly defined subspaces is examined that the wave function "spreads." In effect, it is coarse graining that increases entropy.



(a)



(b)

Fig. 4. Snapshots of an evolving "special" state. Each time step is 0.196 in the units of the model and full decay occurs after 170 time steps ($T \approx 33$). The initial state is that shown in the upper portion of Fig. 3 (so this is a special state for *decay*). (a) From the top, the absolute values of the vector coefficients are shown after 2, 10, and 120 time steps. Note that by time step 10 about half the probability has moved out of the spin-up state and in subsequent time steps sloshes back and forth. (b) Results after 168, 170, and 179 time steps.

also ref. 14). The analogous conclusion could be reached for classical mechanics as well: If a system's evolution is confined to a small torus, the two-time boundary value problem will have many or few solutions, depending on whether the final conditions are on the torus or off it.

Another clue is a refinement of the observation on the number of boson states involved in the "special" states. The initial state, which is all spin up, is expressible in terms of the eigenstates of H. Since under time

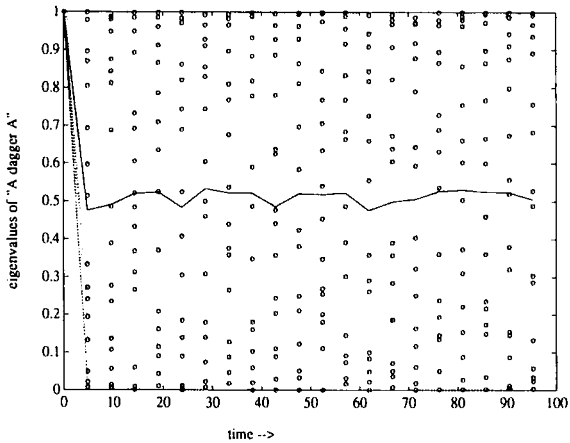


Fig. 5. "Special" states for a 32×32 random Hamiltonian. The space of initial states is defined to be the first 16 dimensions of the Hilbert space.

evolution it does not spread by much, then it did not involve many boson states at time 0. In other words the eigenstates of the full Hamiltonian do not (significantly) involve many boson states and at the same time, using only relatively few of them, one should be able to form a linear combination of unit norm in the half of the Hilbert space defined by P. This was checked taking eigenfunctions of H with eigenvalues near one another and asking whether their projections with P could be used to build vectors of unit or zero norm. The answer turned out to be that if one used about as many vectors as the width of the "special" states, one could approach zero or unit norm closely.[4]

As a further check we looked for "special" states of a random Hamiltonian. It was produced by generating an $N \times N$ array of random numbers uniformly distributed between 0 and 1 and adding this array to its own adjoint. When the first $N/2$ dimensions were arbitrarily designated initial states we actually found no shortage of special states. See Fig. 5. If instead we took fewer dimensions for the initial space, then the nondecay "special" states disappeared (Fig. 6). This is consistent with parameter counting.[6] What is remarkable is that the same reduction of what is considered to be the initial state space does *not* destroy either class of

[4] Mathematically, the search was based on the following: Given a collection of vectors v_k, $k = 1,..., n$, the norm of the largest and smallest vectors constructable as $\sum_k a_k v_k$, with $\sum_k |a_k|^2 = 1$, is given by the largest and smallest eigenvalues of the $n \times n$ matrix whose jk component is given by $v_j^\dagger \cdot v_k$.

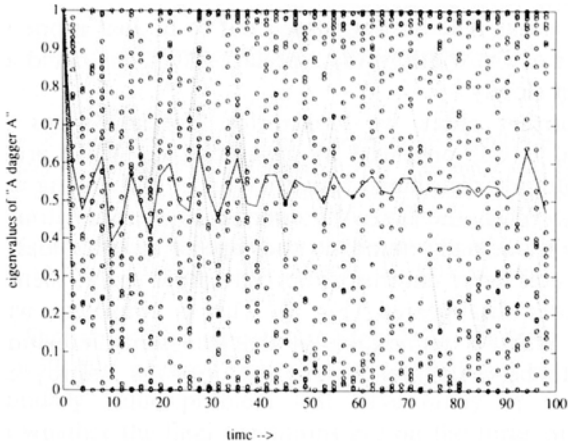


Fig. 6. Same Hamiltonian as Fig. 5, but now only the first 10 dimensions are considered to be the initial states.

"special" states for the spin–boson model. In Fig. 7 we show eigenvalues of B_T for the one-boson Hamiltonian used in the earlier figures when the initial condition space is only considered to be the first 24 dimensions, rather than the 32 dimensions shown earlier (32 being half the total Hilbert space dimension). Thus the spin–boson model gives "special" states even when parameter-counting arguments mitigate against them.

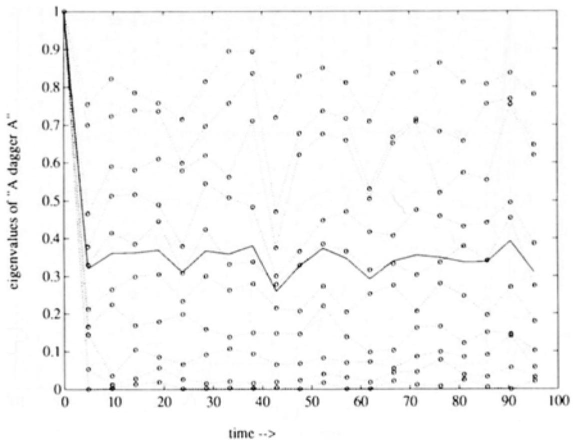


Fig. 7. The 64-dimensional one-boson system of earlier figures, but with the initial states defined to be only the first 24 boson, spin-up dimensions. "Special" states are evident despite the reduced dimension.

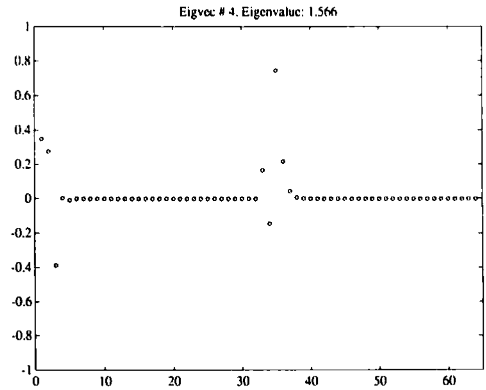


Fig. 8. Representative eigenfunction of the one-boson Hamiltonian used in previous illustrations.

The degree to which evolution spreads the wave function can also be gauged by looking at the eigenfunctions of the Hamiltonian. In Fig. 8 we show an eigenfunction of the one-boson Hamiltonian. This shows remarkable nonspreading of amplitude and is typical of the other eigenfunctions. By contrast the random Hamiltonian eigenfunctions draw amplitude from all the original Hilbert space directions.

6. DISCUSSION

Several questions will be addressed. First there are technical matters, regarding the present results and their possible extension. Then there is the use of these results to support the quantum measurement theory of ref. 1.

At the technical level there are problems that tend to plague computer derivations of decay. In particular, there are plasmonlike collective modes[15] that lead to incomplete decay or early recurrences. These also cut down on "special" state possibilities. The physical significance of these modes is not at present clear.

Another issue is the relation between the existence of "special" states and quantum localization.[6] Under reasonable physical circumstances, parameter counting suggests pessimism for the existence of "special" states. However, when wave functions are confined to relatively small subspaces of Hilbert space—and when these subspaces are those one would naturally use to characterize physical boundary conditions—the parameter counting is transcended and solutions to the two-time boundary value problem are available.

A technical issue with physical significance concerns a spin–boson model with *three* spin states. By considering one spin state ($\otimes$ bosons) to be the initial state and the other two to be distinct decay channels one can address the following question: Can a system with two (or more) decay channels find "special" states so as to decay *only* into one or the other channel?[16] This is in addition to the question of whether there are enough local degrees of freedom to "specialize" the decay to a small time interval (quantum jumps). Exploring this numerically requires large matrices and we do not yet have definitive information. We have found "special" states for decay or nondecay (the latter in defiance of parameter counting), but numerical exploration so far has only turned up states that concentrate their decay up to about 90% into one channel.

In the Introduction we mentioned the relation of "special" states to wave function entanglement. This can be realized by allowing our system to model a capture/noncapture situation. One particle passes near another and they can either bind or continue their separate ways. In both cases there can be excitation of degrees of freedom that are internal or in the environment, e.g., the electromagnetic field. With typical or bland initial conditions a quantum calculation will predict amplitude for both capture and noncapture, so that the final wave function is entangled. Obviously, that could be avoided with "special" states. But one can go beyond this and discuss *dis*entanglement. Two particles bound in an s state are entangled. Generally, if one sends an energetic photon at them it can break up the state—with nonzero, nonunit probability. Thus, with bland initial conditions one does not disentangle, but only becomes more deeply mired in sums of products. However, with further, perhaps environmental, degrees of freedom and the existence of special states, the disentanglement can be implemented with what we termed "pure quantum evolution." The "special" state in this case would be the (time-reversed) end product of the capture event described above.

There is a feature of the "special" states displayed in Sections 4 and 5 that is different from what one ordinarily thinks of as decay states. The system passes from up state to down state and back again. If the down state and its boson excitations truly describe a decayed situation, the return to the up state would be impossible. Often decay modes have translational degrees of freedom that remove them from the region. In fact, in using the spin–boson model to describe Josephson junctions, we find that the possible return to the original state is not only physically possible, but is one of the features of the model (coherent oscillations, etc.). If one wishes, however, to think of this as a model for other decay systems, then the boson modes we deal with are either nontranslational or do not escape from the scene very quickly. In either case, one must justify the existence of these modes in a physical application. It should also be noted that even nontranslational modes can lead to decay (e.g., as in ref. 13) because of a multidimensional final state that does not coherently recombine to the initial state.

We have mentioned two instances where "special" states were not available: at very early times, and when the model parameters were such that decay is severely inhibited, even at long times. In both cases the model is not describing the physics of an observable decay. As is known[17] from the analysis of dominated time evolution (the so-called quantum Zeno effect), observing or measuring decay at early times involves strong coupling of the decaying system to the apparatus that does the measuring. Therefore if one actually were to see decay at those early times, a fully quantum description of that decay would involve the degrees of freedom of the apparatus. In effect, this would mean that the degrees of freedom included in our numerical calculation are *not* all those that are available and in practice not the important ones for decay. Correcting this omission would enable decay and presumably "special" states as well. Similarly, when model parameters are used in which decay is incomplete and inhibited it also does not describe the physics of observed decays and more modes are needed both for the decay and for "special" states.

The investigation described here can easily be taken up on other model systems, for example, rotors, whose localizing properties[18] suggest the presence of "special" states.

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